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1987 J. Phys. A: Math. Gen. 20 L857

(http://iopscience.iop.org/0305-4470/20/13/009)

J. Phys. A: Math. Gen. **20** (1987) L857-L863. Printed in the UK

LETTER TO THE EDITOR

Persistency of two-dimensional self-avoiding walks

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Received 23 April 1987

Abstract. We investigate the persistency of self-avoiding walks on the square lattice by studying the distribution of endpoint displacements, projected in the direction of the first step. Exact enumeration and the constant-fugacity Monte Carlo data indicate that the mean displacement after N steps, $\langle x_N \rangle$, increases logarithmically with N, while the higher odd moments $\langle x_N^{2k+1} \rangle$ vary as $N^{2k\nu} \ln N$, where ν is the correlation length exponent. This unusual behaviour for the moments is found to arise from a simple scaling behaviour of the asymmetric component of the displacement distribution, which in the constant-fugacity ensemble can be written in the form $A(x) \sim \bar{N}^{-2\nu} \ln \bar{N} \exp(-bx/\bar{N}^{\nu})$, where $\bar{N}$ is the average number of steps in the walk at a fixed value of the fugacity and b is a coefficient of order unity.

The salient feature of the self-avoiding walks (SAW) is the infinite memory that they possess as a result of the excluded volume constraint. This infinite memory raises the fundamental question of whether a walk will 'remember' the direction of its initial step as the number of steps, N, tends to infinity. To quantify this 'persistency', one may investigate the N dependence of the mean displacement of the walk after N steps along the direction of the first step, $\langle x_N \rangle$ (figure 1). This problem was first apparently

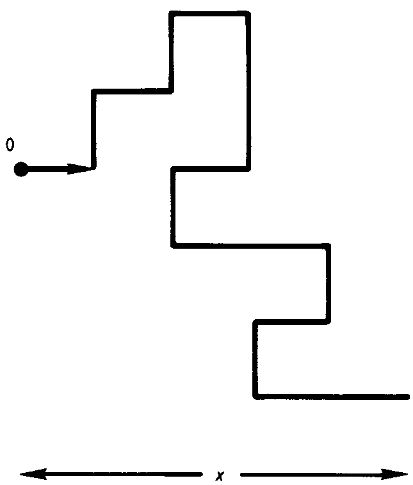

Figure 1. A self-avoiding walk with the first step fixed in the $+x$ direction. The distribution of endpoint displacements along the x axis is measured.

considered by Grassberger (1982), who used exact enumeration to conclude that for SAW in two dimensions $\langle x_N \rangle$ increased as N^w, with $w \simeq 0.063$, although a logarithmic growth in N could not be excluded. This power law growth, if correct, is quite surprising as it indicates that there is a new length scale in the SAW model, independent of the correlation length, which governs how the walk retains memory of its starting direction.

In this letter, we reconsider this persistency problem from the scaling point of view. We have used both exact enumeration and constant-fugacity Monte Carlo simulations to obtain numerical information about the nature of the underlying distribution of endpoint displacements projected along the direction of the first step. We then investigate the behaviour of the odd moments of this distribution, as they provide a natural way of quantifying the asymmetry of the displacement distribution induced by fixing the direction of the first step. These moments are found to exhibit rather unusual behaviour. For the first moment, our analysis suggests that

$$\langle x_N \rangle \sim \ln N \tag{1}$$

while for the odd moments of higher order,

$$\langle x_N^{(2k+1)} \rangle \sim N^{2k\nu} \ln N \tag{2}$$

where ν is the correlation length exponent of the SAW model.

We also address the question of what type of distribution of displacements can yield this peculiar behaviour for the moments. For this purpose, it proves to be useful to decompose the distribution into symmetric, $S(x)$, and antisymmetric, $A(x)$, components, as they govern the behaviour of the even and odd moments, respectively. The antisymmetric component is found to have a surprisingly simple form in the grand canonical ensemble, from which we can account for our numerical data of the moments with very good accuracy. We find that for $x > 0$, $A(x)$ may be written as

$$A(x) \sim \bar{N}^{-2\nu} \ln \bar{N} \exp(-bx/\bar{N}^{\nu}) \tag{3}$$

where $\bar{N} = \langle N(p) \rangle$ is the average value of the number of steps in the walk for a grand canonical ensemble of SAW when the fugacity is equal to p, and b is a constant. Note, however, that $A(x=0)=0$ by construction, so that as a function of the scaled coordinate $x/\bar{N}^{\nu}$, $A(x)$ appears to be discontinuous at the origin.

For concreteness, we consider only SAW on the square lattice in this letter. We first report our numerical results based on enumeration of all walks of up to 24 steps, in which the direction of the first step is kept fixed. Since we record the complete distribution of displacements, any moment of the distribution can be calculated. As indicated in table 1, the behaviour of the odd moments is quite striking. The first moment increases only very slowly with N, and by 24 steps in the walk, $\langle x_N \rangle \sim 2.08$. On the other hand, the higher moments increase at a much faster rate and in fact $\langle x_N^{2k+1} \rangle \gg \langle x_N \rangle^{2k+1}$. Based on rudimentary analyses, the data for $\langle x_N \rangle$ are consistent with a logarithmic growth law, i.e. $\langle x_N \rangle \sim \log N$, while the higher moments appear to obey the scaling behaviour $\langle x_N^{2k+1} \rangle \sim N^{2k\nu}$, where ν is the correlation length exponent of two-dimensional SAW.

In order to understand this unusual behaviour of the moments, and to establish more convincingly the logarithmic behaviour of the first moment, it is important to extend the enumeration data to larger values of N. The constant-fugacity Monte Carlo method is ideally suited for this purpose. In addition, the distribution of displacements takes on an extremely simple form in the constant-fugacity ensemble, while the

Table 1. Enumeration data for the first three odd moments of the distribution of endpoint displacements along the x axis for SAW on the square lattice, when the first step is fixed in the $+x$ direction.

N	$\langle x_N \rangle$	$\langle x_N^3 \rangle$	$\langle x_N^5 \rangle$
2	0.133 33d+01	0.333 33d+01	0.113 33d+02
3	0.144 44d+01	0.677 78d+01	0.414 44d+02
4	0.160 00d+01	0.116 80d+02	0.109 60d+03
5	0.164 79d+01	0.171 97d+02	0.226 44d+03
6	0.173 33d+01	0.240 41d+02	0.418 50d+03
7	0.175 87d+01	0.312 17d+02	0.689 60d+03
8	0.181 74d+01	0.396 92d+02	0.107 83d+04
9	0.183 55d+01	0.483 54d+02	0.157 75d+04
10	0.187 74d+01	0.582 28d+02	0.223 78d+04
11	0.189 21d+01	0.682 39d+02	0.304 16d+04
12	0.192 37d+01	0.793 79d+02	0.405 08d+04
13	0.193 62d+01	0.906 23d+02	0.523 75d+04
14	0.196 12d+01	0.102 93d+03	0.667 49d+04
15	0.197 19d+01	0.115 32d+03	0.832 38d+04
16	0.199 24d+01	0.128 72d+03	0.102 70d+05
17	0.200 16d+01	0.142 18d+03	0.124 62d+05
18	0.201 89d+01	0.156 61d+03	0.149 98d+05
19	0.202 71d+01	0.171 08d+03	0.178 15d+05
20	0.204 19d+01	0.186 49d+03	0.210 24d+05
21	0.204 92d+01	0.201 92d+03	0.245 47d+05
22	0.206 20d+01	0.218 26d+03	0.285 13d+05
23	0.206 86d+01	0.234 60d+03	0.328 26d+05
24	0.208 00d+01	0.251 84d+03	0.376 31d+05

corresponding distribution in the constant-N ensemble arising from enumeration is much more complicated. Moreover, the form of the distribution in the constant-fugacity approach turns out to be very helpful in guiding more detailed analysis of the enumeration data. Thus use of the constant-fugacity ensemble appears to be crucial in elucidating the basic physics of the persistency problem.

The constant-fugacity method generates a grand canonical ensemble of SAW in which the fugacity per step, p, is fixed, while the number of steps in each walk of the ensemble can fluctuate (see, e.g., Redner and Reynolds (1981) and Fisher *et al* (1984) for applications, Dhar and Lam (1986) for a nice explanation of the method, and Berretti and Sokal (1985) for a comprehensive discussion of a related approach). The constant-fugacity approach is closely based on the algorithm used to enumerate SAW: in enumeration, all SAW of up to N steps can be viewed as forming a genealogical tree, in which the nodes represent a particular SAW and the branches represent the ways in which an n-step SAW can grow to $(n+1)$-step SAW by adding a single step. The process of enumeration corresponds to constructing a complete tour on a tree of N levels, in which all nodes are visited.

In the constant-fugacity method, the genealogical tree now has infinitely many levels, as there is no restriction on the number of steps in the walk. However, the enumeration tour is incomplete in that steps in the enumeration algorithm which lead further into the tree are taken with probability p, while steps leading to the root of the tree are still taken with probability unity. This method therefore builds an ensemble with no *a priori* bias, except for that mandated by weighting each step in the SAW by the fugacity. It is worth emphasising that the modifications needed to convert an enumeration program into one that performs constant-fugacity Monte Carlo are trivial if enumeration is based on a tree-like algorithm (Martin 1974, Redner 1982).

As $p \to p_c$ from below, where $p_c \simeq 0.3790\ldots$, the average number of steps in the SAW, $\bar{N} = \langle N(p) \rangle$, diverges as $\gamma p_c(p_c - p)^{-1}$ (Fisher *et al* 1984). Thus by considering a range of p values in the vicinity of p_c, we can study the persistency of long SAW. Typically, fluctuations in $\langle N(p) \rangle$ are extremely small, so that we have written the average number of steps simply as $\bar{N}$ throughout the letter to emphasise that constant-fugacity Monte Carlo serves to extend enumeration data in a meaningful fashion. We have used the constant-fugacity method for p ranging from 0.3 to 0.3735, corresponding to $\bar{N}$ approximately in the range 5–90, to obtain numerical data for the distribution of displacements.

The odd moments in the grand canonical ensemble continue to reflect the striking pattern found in the enumeration data (table 3), namely the first moment grows only very slowly with $\bar{N}$, in a manner consistent with logarithmic growth, while the higher moments all grow at a much faster rate. As mentioned previously, the origin of this behaviour is the surprisingly simple form that the distribution of displacements turns out to possess in the grand canonical ensemble. Let us define $\mathcal{N}(x, p)$ as the (normalised) probability that a SAW ends at a distance x away from its starting point, along the direction of the first step (the $+x$ direction). The symmetric part of this distribution, $S(x, p) = \frac{1}{2}(\mathcal{N}(x, p) + \mathcal{N}(-x, p))$, corresponds to averaging $\mathcal{N}(x, p)$ over the initial step being in the $+x$ and $-x$ directions. This results in a distribution that corresponds closely to the classical probability distribution function of endpoint displacements for SAW.

Table 2. Results of a least-squares fit of $A(x, p)$ to an exponential form, $A(p)\exp(-a(p)x)$, for various values of the fugacity p.

p	$A(p)$	$a(p)$
0.330	0.254	0.370
0.350	0.103	0.240
0.365	0.0320	0.131
0.3675	0.0245	0.112
0.370	0.0210	0.098
0.372	0.0110	0.076
0.3735	0.0093	0.065

On the other hand, the odd moments are determined by the antisymmetric part of the distribution, $A(x, p) = (\mathcal{N}(x, p) - \mathcal{N}(-x, p))$, i.e.

$$\langle x^{2k+1} \rangle = \sum_{x>0} A(x, p) x^{2k+1}. \tag{4}$$

Our numerical data reveal the striking fact that this distribution is a pure exponential function to an excellent approximation for all values of $x > 1$, i.e.

$$A(x, p) \sim A(p)\, \mathrm{e}^{-a(p)x} \tag{5}$$

as illustrated in figure 2. There is a very slight deviation from exponential behaviour at $x = 1$ for the range of fugacities considered here, while the condition $A(x = 0, p) = 0$ is built in. By a standard least-squares fitting procedure, we determined the parameters

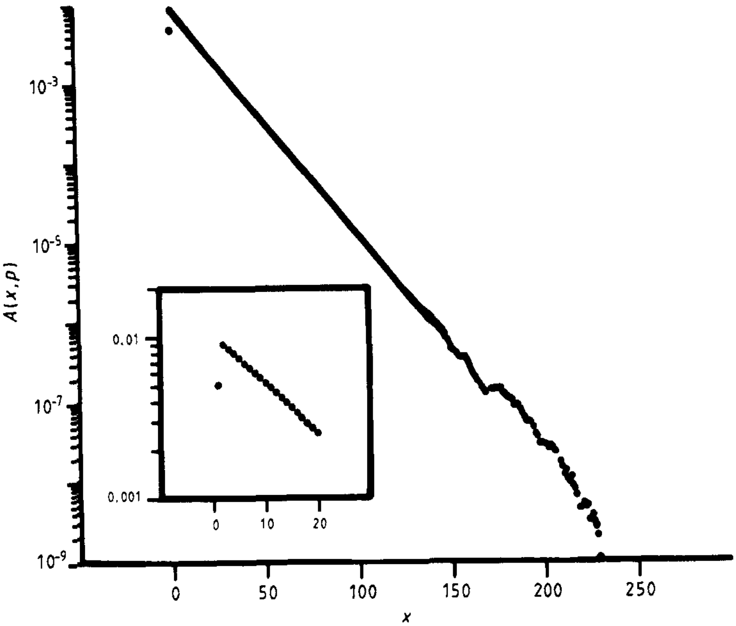

Figure 2. A semilogarithmic plot of the antisymmetric component of the displacement distribution, $A(x, p)$, at fugacity $p = 0.3735$, corresponding to $\bar{N} \simeq 92$. The insert shows details of this distribution near $x = 0$.

$A(p)$ and $a(p)$ as given in table 2. We can then reconstruct phenomenological values of the moments based on this fitted exponential distribution. The comparison between this 'theory' and the actual data is remarkably good, given the very simple assumptions and analysis used for obtaining the fitted distribution for $A(x, p)$ (see table 3).

It now remains to establish the dependence of $A(p)$ and $a(p)$ on $p_c - p$, or equivalently, on $\bar{N}$. Based on plotting these quantities against $p_c - p$ on a double logarithmic scale, and substituting $\bar{N}$ in favour of $(p_c - p)^{-1}$, we find that to a good approximation

$$A(\bar{N}) \sim \bar{N}^{-2\nu} \qquad a(\bar{N}) \sim \bar{N}^{-\nu} \tag{6}$$

where $\nu = 0.75$. If these forms for the parameters in equation (5) are used, one obtains a first moment that is O(1), while the higher moments vary as power laws in $\bar{N}$ (or

Table 3. Comparison of 'theoretical' values for the first three odd moments of the endpoint distribution function based on the fitted exponential form for $A(x, p)$, with the numerical data.

p	$\langle x \rangle_{\mathrm{fit}}$	$\langle x \rangle_{\mathrm{data}}$	$\langle x^3 \rangle_{\mathrm{fit}}$	$\langle x^3 \rangle_{\mathrm{data}}$	$\langle x^5 \rangle_{\mathrm{fit}}$	$\langle x^5 \rangle_{\mathrm{data}}$
0.330	1.85	1.77	81.3	81.6	11 880	12 180
0.350	1.79	1.89	186.3	193.2	64 689	66 288
0.365	1.865	2.06	652.2	668.4	759 840	767 280
0.3675	1.96	2.11	937.8	929.4	1 495 560	1 434 960
0.370	2.19	2.17	1366.2	1344	2 844 720	2 937 960
0.372	1.90	2.23	1978.2	2118	6 850 080	6 987 000
0.3735	2.20	2.30	3126	3162	14 797 320	15 150 000

$p_c - p$). Thus to obtain a more complete representation for the moments either A or a, or perhaps both quantities, must be modified by a logarithmic correction factor. Unfortunately, the Monte Carlo data for A and a are not sufficiently accurate to permit the detection of a logarithmic correction factor directly. However, if A contained a single factor of $\ln \bar{N}$, then $\langle x_N \rangle \sim \ln \bar{N}$, consistent with the available data, while $\langle x_N^{(2k+1)} \rangle \sim \bar{N}^{2k\nu} \ln \bar{N}$. On the other hand, if there were a logarithmic correction to a instead (or in addition), then the higher moments would be each modified by different powers of $\ln \bar{N}$.

We therefore reconsider the enumeration data in order to ascertain the possible existence of such logarithmic correction factors. To this end, we have examined the series for various moment ratios. It appears that the most useful test is obtained by studying the series $y(N, k) = \langle x_N^{(2k+1)} \rangle / (\langle x_N^{(2k-1)} \rangle \langle x_N^2 \rangle)$. If $\langle x_N^{(2k+1)} \rangle$ scales as $N^{2k\nu} \ln N$, then as $N \to \infty$, the $y(k, N)$ will approach a limiting k-dependent value y_k. On the basis of various Nevill-type extrapolations for the $y(k, N)$, this indeed appears to be the case. We also find that the y_k appear to fit the simple relation $y_k = (9+k)/4$ to within an accuracy of several per cent, up to $k = 11$. Although this analysis for logarithmic correction factors is not definitive, it does suggest that only the parameter A in equation (5) is multiplied by single power of the logarithm of $\bar{N}$. We therefore propose that the asymmetric component of the displacement distribution has the form written in equation (3), and this accounts for most of the features of our numerical data.

It is worth pointing out that the persistency phenomenon observed in the SAW model appears in almost the same form for other related stochastic walk models. For example, for pure random walks with no excluded-volume constraint, a system corresponding to the SAW persistency problem may be defined by considering a random walk which starts out one lattice spacing away from a site which is a perfect trap. This trapping site plays precisely the same role as the fixed starting direction in the SAW model. For this random walk problem in two dimensions, Weiss (1981) has shown that $\langle x_N \rangle$ increases logarithmically in N, while the higher moments increase as a power law in N. Furthermore, there also appears to be a multiplicative logarithmic correction to the higher moments (Weiss 1987), so that the overall behaviour is closely analogous to that found for the SAW problem.

Another instructive example, where the persistency can actually be solved exactly, is the case of a partially directed SAW (Fisher and Sykes 1959). For example, consider a two-dimensional model in which the allowed step directions are either $+y$ or $\pm x$, and in which the first step is specified to be in the $+x$ direction. For this model, an explicit calculation shows that $\langle x_N \rangle \to 1 + 1/\sqrt{2}$ as $N \to \infty$. In addition, both the second and third moments of the displacement vary linearly with N, and it is possible to convince oneself that an analogous pattern of behaviour continues for the higher moments. In this case, the behaviour is similar to the conventional SAW model, except that the logarithmic factors in the moments are missing.

In conclusion, we have studied the persistency of two-dimensional self-avoiding walks induced by fixing the direction of the first step. On the basis of enumeration and constant-fugacity Monte Carlo data, we have shown that the first moment of the displacement along the direction of the initial step grows logarithmically with N, while the higher odd moments grow as a power law in N. This behaviour arises from a simple exponential form for the antisymmetric component of the distribution of projected endpoint displacements in the constant-fugacity ensemble. The unusual behaviour found here suggests that it will be interesting to consider the persistency of self-avoiding walks in greater than two dimensions.

We thank P Grassberger and G H Weiss for communicating useful results relevant to the persistency problem. Research by VP has been supported by the US National Science Foundation under grant DMR-86-01208, and by the Donors of the Petroleum Research Fund, administered by the American Chemical Society, under grant ACS-PRF-18175-G6. The Center for Polymer Studies is supported in part by grants from the ARO, NSF and ONR. This financial assistance is gratefully acknowledged.

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